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Mercury Cadmium Telluride (MCT) has a very large electron mobility and exhibits a non-ohmic behavior in relatively small electric fields. The goal of this project was to reach the understanding of electron transport properties of narrow band gap semiconductors, with emphasis on high-field behavior. Even though the primary material of interest was Mercury Cadmium Telluride (MCT), but we also investigated Indium Antimonide.

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Researchers derived expressions for scattering rates for electrons in Mercury Cadmium Telluride which accounted for correct wave functions for narrow band gap materials, and performed the Monte-Carlo simulation of $Hg_{0.205}Cd_{0.795}Te$ at 77K for different doping levels.

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B. Gelmont, B. Lund, K. Kim, G. Jensen, M. Shur, and T. Fjeldly, "Monte Carlo simulation of Mercury Cadmium Telluride", Journal of Applied Physics, vol. 71, No. 10, pp. 4977-82 (1992)

B. Gelmont, K.-S. Kim, M. Shur."Doping Dependence of Breakdown Field in Mercury Cadmium Telluride" , International Workshop on Computational Electronics, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign (1992)

B. Gelmont, K. S. Kim, M. Shur, "Theory of Impact Ionization and Auger Recombination in $Hg_{1-x}Cd_xTe$", Physical Review Letters, vol. 69, No.8, pp. 1280-2 (1992)

B. Gelmont, K. S. Kim, and M. Shur, "Monte Carlo Calculation of Electron Transport in Gallium Nitride", J. Appl. Phys., 74 (3), pp. 1818-1821, 1 August (1993)

M. Shur, W. C. B. Peatman, B. Gelmont, K.Lee, "Novel Semiconductor Devices for High Speed VLSI and Ultra-High Frequency Applications", International Conference on VLSI and CAD (ICVS 93),pp. 442-9,Taejon,Korea,November 15-17,1993

M. Shur, B. Gelmont, C. Saavedra-Munoz, and G. Kelner, "Potential of Wide Band Gap Semiconductor Devices for High Temperature Applications, in Proceedings of 5th International Conference on Silicon Carbide and Related Compounds", Invited, to be published

Submitted for publication:
B. Gelmont, M. Shur, and M. Stroscio, "Polar Optical Phonon Scattering in Three and Two Dimensional Electron Gases" submitted to J. Appl. Phys.

8. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT:

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BRIEF OUTLINE OF RESEARCH FINDINGS

Mercury Cadmium Telluride (MCT) has a very large electron mobility and exhibits a non-ohmic behavior in relatively small electric fields. The goal of this project was to reach the understanding of electron transport properties of narrow band gap semiconductors, with emphasis on high-field behavior. Even though the primary material of interest was Mercury Cadmium Telluride (MCT), but we also investigated Indium Antimonide. We derived expressions for scattering rates for electrons in Mercury Cadmium Telluride which accounted for correct wave functions for narrow band gap materials. We performed the Monte-Carlo simulation of $Hg_{0.205}Cd_{0.795}Te$ at 77K for different doping levels. First, we studied how the electric field influences the screening length. To adopt time varying impurity screening length and to account for the Pauli exclusion principle, we updated the distribution function, the screening length, and scattering rate table each 140 fsec, by collecting data from all carriers during this time interval. The screening length increases with the electric field due to the increase of the average electron energy.

The simulation results with and without taking into account the Pauli exclusion principle and time varying screening length showed that for $n=5.4x10^{15}$ cm^{-3}, the more accurate method reduces the electron velocity by 5-10% depending on the electric field. Thus adopting the Pauli exclusion principle and time varying screening length is required for high carrier concentration. We also computed the dependence of the low field mobility on the electron concentration at 77K.

The impact ionization in MCT becomes important in relatively small electric fields because of the low ionization threshold energy and large electron mobility. Experimental data show that the impact ionization dramatically affects the current-voltage characteristics of the Hg_{1-x} Cd_xTe (x ~ 0.2) at ~250 V/cm.

The understanding of the impact ionization phenomenon and, especially, the calculation of the impact ionization rates and current-voltage characteristics under impact ionization conditions is a difficult task because it involves the hot carriers at the energies corresponding to the distribution tail. At such high energies, even the details of the band structure are not usually known with a

sufficient degree of accuracy for a quantitative description of the impact ionization, and the band structure cannot be readily described by analytical expressions. This is compounded by numerical difficulties of the calculation of the distribution tail. These difficulties can be successfully resolved for Narrow Gap Semiconductors (NGS) such as MCT ($Hg_{1-x}Cd_xTe$ ($x \sim 0.2$)). In these semiconductors, the band gap E_g is much smaller than the intervalley separation energies. As a result all processes related to hot electrons are confined to the central valley where the electron wave function and dispersion law can be described in the frame of the Kane model. This allowed us to derive analytical expressions for the impact ionization rate and for the rate of the so-called Conduction band - Conduction band -Heavy hole band - Conduction band (CCHC) Auger process. However the overlap integrals between the heavy hole and electron wave functions, calculated in the frame of the Kane model, vanish for the threshold momenta of particles . Hence, the overlap integral in NGS is anomalously small at the threshold. Only the interaction with other bands gives a nonzero contribution to the overlap integrals. This is why the standard theory of the impact ionization rate has to be revised for NGS, and the energy dependence of the overlap integrals has to be taken into account. We derived equations for the impact ionization rate and the coefficient of the CCHC Auger process. We used an ensemble Monte-Carlo simulation in order to determine the electron distribution function, the average electron energy, and drift velocities in an electric field.

After this calculation, the excess carrier concentration was found from the particle balance. Multiplying the carrier concentration by the electron drift velocity, we obtained the current-voltage characteristics which we compared with experimental data. A very good agreement with the experimental data confirmed the validity of our approach which can be used for the calculation of the ionization and Auger recombination rates in NGS and which is simple enough to be implemented in device simulation programs.

Also, our results appear to have relevance for wide band gap semiconductors as well. In our previous study, we have calculated transport properties using Monte Carlo simulations as well as numerical calculations .

Our second goal was to derive simple analytical equations for the electron mobility. One of fundamental difficulties for developing such an approach was an impossibility to utilize the relaxation time approximation when the electron thermal energy is comparable or smaller than the optical phonon energy. However the relaxation time approximation can be introduced when the electron thermal energy is much smaller than the optical phonon energy if we consider two-step collision process (absorption/emission). In this process, a low energy electron absorbs a phonon and then almost immediately the phonon emission occurs. The electron energy will be almost the same after these two successive scattering processes. We derived an analytical equation for the polar optical phonon mobility which is valid when the electron thermal energy is much smaller than the optical phonon energy. We compared our analytical calculation with the Monte-Carlo simulation of the velocity field characteristic and diffusivity for InSb at 77 K and obtained a very good agreement. We also took into account the effects of the nonparabolicity which include the change of the dispersion law and the interband mixing of wave functions. We calculated the polar optical phonon mobility of the 2D-gas near insulator-semiconductor heterostructure in Metal-Insulator-Semiconductor (MIS) structure. As mentioned above, our results also found application in the Monte Carlo simulation of wide band gap semiconductors.